Integrated density of states of Schrödinger operators with periodic or almost-periodic potentials

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Joint work with Roman Shterenberg (Birmingham Alabama)
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acting in \( \mathbb{R}^d \). The potential \( b = b(x) \) is assumed to be real, smooth, and either periodic, or almost-periodic. The density of states of \( H \) can be defined by the formula

\[ N(\lambda) = N(\lambda; H) := \lim_{L \to \infty} \frac{N(\lambda; H^{(L)}_D)}{(2L)^d}. \]

Here, \( H^{(L)}_D \) is the restriction of \( H \) to the cube \([-L, L]^d\) with the Dirichlet boundary conditions, and \( N(\lambda; A) = \#\{\lambda_j(A) \leq \lambda\} \) is the counting function of the discrete spectrum of \( A \).
To begin with, let us assume that the potential \( b \) is periodic with lattice of periods \( \Gamma \). Let \( \Gamma^\dagger \) be the dual lattice to \( \Gamma \). Then we can perform Floquet-Bloch decomposition and express the operator \( H \) as a direct integral

\[
H = \int_\oplus H(\mathbf{k}) d\mathbf{k},
\]

quasi-momentum \( \mathbf{k} \) running over \( \mathbb{R}^d / \Gamma^\dagger \). Here, \( H(\mathbf{k}) = (i\nabla + \mathbf{k})^2 + b \) acting in \( L^2(\mathbb{R}^d / \Gamma) \). Then we can express the density of states as

\[
N(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d / \Gamma^\dagger} N(\lambda, H(\mathbf{k})) d\mathbf{k}.
\]
If we put $H_0 = -\Delta$, for positive $\lambda$ we have

$$N(\lambda; H_0) = C_d \lambda^{d/2},$$

where

$$C_d = \frac{w_d}{(2\pi)^d}$$

and

$$w_d = \frac{\pi^{d/2}}{\Gamma(1 + d/2)}$$

is a volume of the unit ball in $\mathbb{R}^d$. 
There is a long-standing conjecture that the density of states of $H$ enjoys the following asymptotic behaviour as $\lambda \to \infty$:

$$N(\lambda) \sim \lambda^{d/2} \left( C_d + \sum_{j=1}^{\infty} e_j \lambda^{-j} \right),$$

meaning that for each $K \in \mathbb{N}$ one has

$$N(\lambda) = \lambda^{d/2} \left( C_d + \sum_{j=1}^{K} e_j \lambda^{-j} \right) + R_K(\lambda)$$

with $R_K(\lambda) = o(\lambda^{\frac{d}{2} - K})$. 
The coefficients $e_j$ are real numbers which depend on the potential $b$. They can be calculated using the heat kernel invariants, computed by Polterovich, Hitrik-Polterovich, and Korotyaev-Pushnitski; they are equal to a certain integrals of the potential $b$ and its derivatives. For example,

$$e_1 = -\frac{d w_d}{2(2\pi)^d|\mathbb{R}^d/\Gamma|} \int_{\mathbb{R}^d/\Gamma} b(x) dx$$

and

$$e_2 = \frac{d(d-2)w_d}{8(2\pi)^d|\mathbb{R}^d/\Gamma|} \int_{\mathbb{R}^d/\Gamma} (b(x)^2) dx.$$
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If $d \geq 3$, only partial results are known, works by Skriganov, Karpeshina, Helffer, Mohamed, Veliev, Sobolev, Knörrer, Trubowitz, L.P.

In particular, Yu.Karpeshina showed that when $d = 3$, formula (2) is valid with $K = 1$ and $R(\lambda) = O(\lambda^{-\delta})$ with some small positive $\delta$ and $R(\lambda) = O(\lambda^{d-3/2} \ln \lambda)$ when $d > 3$. 
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If $b$ is almost-periodic and $d = 1$, formula (1) was proved by Savin (1988). For $d \geq 2$, (2) is known only with $K = 0$ and $R(\lambda) = O(\lambda^{\frac{d-2}{2}})$ (Shubin, 1987).
Theorem.

*Formula (1) is valid for smooth periodic $b$ and arbitrary $d$.***
Let $b$ be either quasi-periodic:

$$b(x) = \sum_{\theta \in \Theta} a_\theta e^{i\theta x}$$

($\Theta$ being a finite set), or almost-periodic (a uniform limit of quasi-periodic functions).
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$$M(b) := \lim_{L \to \infty} \frac{\int_{[-L,L]^d} b(x) dx}{(2L)^d}$$

exists and is called the mean of $b$. 
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$$\mathbf{M}(b) := \lim_{L \to \infty} \frac{\int_{[-L,L]^d} b(x) dx}{(2L)^d}$$

exists and is called the mean of $b$. For each $\theta \in \mathbb{R}^d$ we define the Fourier coefficient

$$a_\theta = a_\theta(b) := \mathbf{M}_x(b(x)e^{-i\theta x})$$

and the spectrum $\Theta(b) := \{ \theta \in \mathbb{R}^d, a_\theta \neq 0 \}$. 
Each almost-periodic function has a (formal) Fourier series

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For a set \( S \subset \mathbb{R}^d \) by \( Z(S) \) we denote the set of all finite linear combinations of elements in \( S \) with integer coefficients.

Condition A. Suppose that \( \theta_1, \ldots, \theta_d \in Z(\Theta) \). Then

\[ Z(\theta_1, \ldots, \theta_d) \]

is discrete. This condition can be reformulated like this: suppose, \( \theta_1, \ldots, \theta_d \in Z(\Theta) \). Then either \( \{\theta_j\} \) are linearly independent, or

\[ \sum_{j=1}^{d} n_j \theta_j = 0, \]

where \( n_j \in \mathbb{Z} \) and not all \( n_j \) are zeros.

Theorem. Formula (1) is valid for quasi-periodic \( b \) satisfying Condition A.
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**Theorem.**

*Formula (1) is valid for quasi-periodic b satisfying Condition A.*
Suppose, $b$ is almost-periodic. Let $k \in \mathbb{N}$ be arbitrary. We require that for each sufficiently small $\epsilon$ there exists a quasi-periodic potential

$$\tilde{b}(x) = \sum_{\theta \in \tilde{\Theta}} \tilde{a}_\theta e^{i\theta x}$$

so that

$$||b - \tilde{b}||_\infty < \epsilon.$$ 

Let $\tilde{\Theta}_k := \tilde{\Theta} + \tilde{\Theta} + \cdots + \tilde{\Theta}$ (algebraic sum taken $k$ times). We require $\sup_{\theta \in \tilde{\Theta}_k} |\theta| \ll \epsilon^{-1/k}$, $\inf_{\theta \in \tilde{\Theta}_k, \theta \neq 0} |\theta| \gg \epsilon^{1/k}$. We also require that the angles between all subspaces spanned by elements of $\tilde{\Theta}_k$ are bounded below by $C\epsilon^{1/k}$.

Let $\theta_1, \ldots, \theta_m \in \tilde{\Theta}_k$, $m < d$. Denote by $\mathcal{V}$ the linear span of these vectors and put $\Gamma_{\mathcal{V}} := \mathbb{Z}(\tilde{\Theta}_k \cap \mathcal{V})$. Condition A implies that $\Gamma_{\mathcal{V}}$ is discrete. Our final requirement is: $|\mathcal{V}/\Gamma_{\mathcal{V}}| \gg \epsilon^{1/k}$.

**Theorem.**

*Formula (1) is valid for almost-periodic $b$ satisfying Condition A and all the above conditions.*
The coefficients are computed by similar formulas, e.g.

\[ e_1 = -\frac{d w_d}{2(2\pi)^d} M(b) \]

and

\[ e_2 = \frac{d(d - 2) w_d}{8(2\pi)^d} M(b^2) \]
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Actually, we prove the following formula:

\[ N(\rho^2) = C_d \rho^d + \sum_{p=0}^{d-1} \sum_{j=-d+1}^{K} e_{j,p} \rho^{-j}(\ln \rho)^p + o(\rho^{-K}) \],

but most of the coefficients turn out to be zero due to Hitrik-Polterovich.
What is the analogue of the formula

\[
N(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d / \Gamma^\dagger} N(\lambda, H(k)) \, dk
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for almost-periodic \( b \)? There are two definitions, and we need them both!
What is the analogue of the formula

\[ N(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d / \Gamma^+} N(\lambda, H(k)) dk \]

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Definition 1:
In all points of continuity of \( N \), we have:

\[ N(\lambda) = M_x(e(\lambda; x, x)) \]

where \( e(\lambda; x, y) \) is the integral kernel of the spectral projection of \( H \).
Definition 2 (cheating)

\[ N(\lambda) = T(E_\lambda(\tilde{H})) = D(E_\lambda(\tilde{H})L^2(\mathbb{R}^d)). \]

Here, \( T \) is the regularized (von Neumann) trace, and \( D \) is the relative dimension.
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In particular, \( N(\lambda; H) = N(\lambda; U^{-1}HU) \), where \( U \) is a unitary operator with almost-periodic coefficients.
Another useful trick: often, we work with operators acting not in $L_2(\mathbb{R}^d)$, but in $B_2(R^d)$ (Besicovitch space). This is a collection of all formal sums

$$\sum_j a_j e^{i\theta_j x}$$

with

$$\sum_j |a_j|^2 < +\infty.$$

This is a non-separable Hilbert space. Results of Shubin show that the norms and spectra of almost-periodic operators acting in $L_2(\mathbb{R}^d)$ and $B_2(R^d)$ are often the same.
Assume now for simplicity that $b$ is periodic. There are two methods of obtaining information of the eigenvalues of $H(k)$. The first method is called the method of spectral projections. Let $\{P_j\}$ be spectral projections of $H_0$ (i.e. they are projections commuting with $H_0$) so that $\sum P_j = I$. We look at the operator

$$\tilde{H} = \sum_j P_j HP_j.$$ 

If we choose the projections $P_j$ very carefully, then the spectra of $H$ and $\tilde{H}$ are close to each other.

The second method is called the method of gauge transform. We look at the operator $H_1 = e^{-i \Psi} H e^{i \Psi}$. After carefully choosing bounded pseudo-differential almost-periodic operator $\Psi$, we can achieve that $H_1$ is norm-close to the operator $H_2$ which is 'almost' diagonal and so has many invariant subspaces.
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After carefully choosing bounded pseudo-differential almost-periodic operator $\Psi$, we can achieve that $H_1$ is norm-close to the operator $H_2$ which is ‘almost’ diagonal and so has many invariant subspaces.
Both methods produce two types of invariant subspaces (of $\tilde{H}$ or $H_2$): stable (corresponding to perturbations of simple eigenvalues, lying not too close to other eigenvalues) and unstable (corresponding to perturbations of a cluster of eigenvalues lying close together). It is straightforward to compute the contribution to the density of states from the stable subspaces. Unstable eigenvalues cause the main problem.
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$$r^2 I + S(r),$$

where $r \sim \lambda^{1/2}$ and $S(r)$ is a self-adjoint finite-dimensional operator with (almost explicitly written) analytic symbol.
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We can use the expansion

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\lambda(A + \epsilon B) \sim \sum \lambda_j \epsilon^j,
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but we cannot integrate it against \( dk \), since the coefficients \( \lambda_j \) can be unbounded functions of \( k \).
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In our previous paper, we have shown that if $d = 2$, we have

$$\lambda(A + \epsilon B) \sim \sum \epsilon^j \lambda_j \pm \sqrt{\sum \epsilon^j \tilde{\lambda}_j},$$

where the coefficients $\lambda_j$ and $\tilde{\lambda}_j$ are bounded functions of the quasi-momentum and so can be integrated against $dk$. 
Now we use the method of gauge transform. Then $S(r)$
does not have a nice form, but we need to compute the
contribution from all eigenvalues of $r^2 I + S(r)$, whereas
before we had to separate the eigenvalues contributing to
the density of states from the rest of eigenvalues. Since
$\|S'(r)\| < r/2$, each eigenvalue $\lambda_j(r^2 I + S(r))$ is an
increasing function of $r$. Thus, the equation

$$r^2 + \lambda_j(S(r)) = \lambda =: \rho^2$$

has a unique solution, denoted by $\tau_j$. The contribution to
the density of states equals

$$\sum_j \tau_j^m,$$

where $m \in \mathbb{N}$. 
Let $\gamma$ be a contour in the complex plane containing all points $\tau_j$. The points $\tau_j$ are singularities of $\det[S(z) + z^2 I - \rho^2 I]$. Using

$$\text{tr}[F'(z)F^{-1}(z)] = (\det[F(z)])'(\det[F(z)])^{-1}$$

and the residue theorem, we obtain:
\[
\sum_j \tau_j^m = \frac{1}{2\pi i} \oint_\gamma z^{m+1} (\det[S(z) + z^2 I - \rho^2 l])' (\det[S(z) + z^2 I - \rho^2 l])^{-1} \, dz \\
= \frac{1}{2\pi i} \oint_\gamma \text{tr}[z^{m+1} (2zl + S'(z))(S(z) + z^2 I - \rho^2 l)^{-1}] \, dz \\
= \frac{1}{2\pi i} \oint_\gamma \text{tr}[(2z^{m+2} I + z^{m+1} S'(z))(z^2 - \rho^2)^{-1} \sum_{l=0}^{\infty}(-1)^l S^l(z)(z^2 - \rho^2)^{-l}] \, dz \\
= \frac{1}{2\pi i} \sum_{l=0}^{\infty} (-1)^l \oint_\gamma \text{tr}[(2z^{m+2} I + z^{m+1} S'(z))S^l(z)(z - \rho)^{-(l+1)}(z + \rho)^{-(l+1)}] \, dz \\
= \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} \text{tr} \left. \frac{d^l}{dr^l} [(2r^{m+2} I + r^{m+1} S'(r))S^l(r)(r + \rho)^{-(l+1)}] \right|_{r=\rho}.
\]